Spreading and annihilating particles: surprises from mean-field theory

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Abstract

We study the pairwise annihilation process $A+A \rightarrow$ inert of a number of random walkers, which originally are localized in a small region in space. The size of the colony and the typical distance between particles increases with time and, consequently, the reaction rate goes down. In the long time limit the spatial density profile becomes scale invariant. The mean-field approximation of this scenario bears some surprises. It predicts an upper critical dimension $d_c = 2$, with logarithmic corrections at the critical dimension and nontrivial scaling behavior for $d < 2$. Based on an exact solution of the one dimensional system we conjecture that the mean-field *exponents* are in fact correct even below the upper critical dimension, down to $d = 1$, while the corresponding scaling function that describes the spatial density profile, changes for $d < 2$ due to the stochastic fluctuations.

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Recently there has been much progress made in the understanding of the kinetics of diffusing and reacting particles. In particular, the evolution of spatial patterns in chemical and biological systems has been subject to intensive research for many years. The effects of (chemical) reactions between diffusively spreading particles, or of ecological competition on a spreading population of species (in the absence of convection) can often be described by a reaction diffusion equation of the type

$$\partial_t \mathbf{n} = \mathbf{D}\nabla^2 \mathbf{n} + \mathbf{f}(\mathbf{n}) \tag{1}$$

where $\mathbf{n}(\underline{x}, t)$ is the vector of reactants, $\mathbf{D}$ is a matrix of diffusivities, and $\mathbf{f}(\mathbf{n})$ describes the nonlinear reaction kinetics [1]. Equation (1) is really a deterministic approximation ('mean-field'-approximation) of the underlying

stochastic process, replacing the discrete and fluctuating occupation numbers of the particles by a continuous (coarse grained) population density. In this paper we show that for the specific case of a single species of diffusing particles A that annihilate each other upon contact $A+A \to$ inert, and for a certain set of (localized) initial conditions, this mean-field approximation is surprizingly powerful: it yields the correct scaling exponents in all dimensions, even down to $d \geq 1$, while for $d < 2$ the stochastic fluctuations due to the discreteness of the process change only the corresponding scaling function. Generally, in contrast, mean field theory is expected to yield exact scaling exponents only *above* the upper critical dimension (which is 2 in this case), wheras below, the stochastic fluctuations lead to anomalous exponents. Right at the critical dimension we usually find logarithmic corrections to the mean-field behavior.

For stochastically *homogeneous* initial conditions, for example, the $A + A \to$ inert reaction [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12] (and the closely related reaction $A + A \to A$, where particles undergo a Brownian motion until they hit another particle and undergo coagulation rather than annihiliation, which is described by the same mean-field equation as the $A + A \to$ inert process) the density decays as $n \sim t^{-d/2}$ for dimensions below the critical dimension $d_c = 2$, and as $n \sim 1/t$ for $d > 2$. The latter formula can be deduced from the deterministic ("mean-field") equation of motion for the coarse-grained spatial density $n(\underline{x}, t)$

$$\partial_t n = \nabla^2 n - n^2, \tag{2}$$

where we have absorbed the diffusion constant and the reaction rate into the time and length scale. The ∇^2-term describes again the diffusion of the particles, whereas the n^2-term accounts for the pairwise annihilation process. For a homogeneous density the mean-field equation reduces to $\dot{n} = -n^2$ leading to $n \sim 1/t$.

For a certain set of localized initial conditions, however, there is an exception to the general change in behavior below the upper critical dimension, due to the simple renormalization-group properties of the $A + A \to$ inert-reaction [4]. In this case the mean-field equation (2) itself predicts correct exponents, the upper critical dimension and logarithmical corrections: at the beginning the system shall be empty up to a finite, populated region. From this region particles will spread into the 'vacuum' due to the diffusive motion of the particles; and for asymptotically long times we find a scale invariant density profile. We will calculate this profile within the mean-field approximation and compare it with an exact solution of the one-dimensional problem.

The system under consideration serves as a toy model for systems displaying a diffusive spreading of reacting agents from a localized region into

space, e.g. models for chemical reactions which are ignited at some point. It is related to but should not to be confused with the much more complicated directed percolation problem [13, 14, 15] where, starting from a localized seed, particles can split, react, die and move diffusively.

A one-dimensional lattice version of the $A + A \to$ inert-reaction with a homogeneous initial state was solved exactly [5, 9, 10, 11, 12, 16] owing to the fact that the stochastic matrix which enters the master equation can be expressed as a bilinear form of fermionic operators. The mean density was found to decay as $n \sim t^{-1/2}$. In addition, correlation functions were derived [9, 10, 11], confirming the picture of a critical, non equilibrium system with anomalous exponents. For dimensions $d > 1$, an exact RG-approach [4, 7, 8, 17] established the upper critical dimension $d_c = 2$ and the power law $n \sim t^{-d/2}$ for dimensions $d < 2$. Consequently, the typical distance ℓ between particles grows like the diffusion length $\ell \sim \sqrt{t}$. This can be understood from the recurrence property of random walks for $d \leq 2$: Within a time intervall t a Brownian particle reacts with particles at distances smaller than the diffusion length ℓ, leaving behind voids of linear size $\sim \ell$ [2, 18, 19].

In order to solve the mean-field equation (2) we substitute

$$n(\underline{x}, t) = \frac{1}{t}\phi\left(\frac{\underline{x}}{\sqrt{t}}, t\right), \tag{3}$$

reflecting the naive dimensions of time, length and the density n. It should be kept in mind, that this substitution is without loss of generality. Plugging (3) into (2) yields ($\underline{r} = \underline{x}/\sqrt{t}$ is the rescaled position)

$$t\partial_t\phi(\underline{r}, t) = \nabla_r^2\phi + \frac{1}{2}\nabla_r \cdot (\underline{r}\phi) + (1 - d/2)\,\phi - \phi^2. \tag{4}$$

Introducing a logarithmical time variable $s = \log(t/t_0)$, where t_0 is an arbitrary time scale, we arrive at

$$\partial_s\phi(\underline{r}, s) = \nabla^2\phi + \frac{1}{2}\nabla \cdot (\underline{r}\phi) + (1 - d/2)\,\phi - \phi^2, \tag{5}$$

which looks similar to the original equation of motion with, however, a deeply modified propagator (linear part). We linearize equation (5) in ϕ and split it into

$$\partial_s\phi = \Omega\phi + (1 - d/2)\phi, \tag{6}$$

where the operator Ω, defined through $\Omega\phi = \nabla^2\phi + (1/2)\nabla \cdot (\underline{r}\phi)$ has zero or negative eigenvalues. The unique groundstate (zero mode) of Ω is $\phi_0 = \exp(-r^2/4)$; the other eigenfunctions $\phi_{n_1,\ldots,n_d} = \partial_1^{n_1} \ldots \partial_d^{n_d}\phi_0$ correspond to negative eigenvalues $\lambda = -(n_1 + \ldots + n_d)/2$ (using the notation $\partial_i \equiv \partial/\partial r_i$).

A critical dimension $d_c = 2$ separates two qualitatively different sectors: the linearized equation (6) shows a growing mode for $1 \leq d < 2$, whereas all modes are exponentially damped in s for $d > 2$. For $1 \leq d < 2$ and a nonzero localized initial condition, the unstable mode of ϕ will grow until it saturates due to the presence of the nonlinear term. There is a unique, stationary state ϕ^* of (6), given by $\nabla^2\phi^* + (1/2)\nabla \cdot (\underline{r}\phi^*) + (1 - d/2)\phi^* - (\phi^*)^2 = 0$. A closer inspection reveals that ϕ^* is stable, positive, has spherical symmetry and decays faster than any power for $r \to \infty$. Going back to the original coordinates via (3), we obtain the asymptotic time dependence of the density $n(\underline{x}, t) = t^{-1}\phi^*(\underline{x}/\sqrt{t})$. Consequently, in $d < 2$, the long time decay of the total number of particles, for localized initial conditions is given by

$$N = \int d^d x \; n(\underline{x}, t) \sim t^{d/2-1}, d < 2. \tag{7}$$

For $d = 2$ we see in fact logarithmic terms. The linearized equation (6) has a marginal mode (zero mode) ϕ_0. Therefore the time dependence of its amplitude A is governed by the nonlinear term: $\partial_s A \propto -A^2$ yielding $A \sim 1/s = 1/\log(t/t_0)$. Consequently, the total number of particles is not constant as a naive extrapolation of (7) would suggest, but vanishes according to $N \sim 1/\log(t/t_0)$. For dimensions above the critical dimension and a localized initial condition, ϕ behaves like $\phi \sim \exp((1 - d/2)s - r^2/4)$ as beeing the slowest mode of the linearized equation (6). The nonlinearity turns out to be irrelevant since ϕ^2 will vanish twice as fast as ϕ. Using the original coordinates, we have $n(\underline{x}, t) \sim t^{-d/2} \exp(-x^2/(4t))$, i.e. simple diffusion with a conserved total number of particles. In fact, for dimensions $d \leq 2$ two particles meet with probability one, whereas for dimensions $d > 2$ two widely separated particles will miss each other and survive.

The remainder of this letter is devoted to an exact solution of the stochastic one-dimensional system along the lines of [5, 9, 10, 11, 12]. We represent an occupied site $i = \ldots, -1, 0, 1, 2, \ldots$ by an occupation number $\tau_i = 1$ and an empty site by $\tau_i = 0$. We start with the initial condition:

$$\begin{array}{rccccccccccc} \text{initial state:} & \ldots & 0 & 0 & 1 & 1 & \ldots & 1 & 1 & 0 & 0 & \ldots \\ \text{site:} & \ldots & -1 & 0 & 1 & 2 & \ldots & L-1 & L & \ldots, & & \end{array} \tag{8}$$

where we choose an even number of occupied sites L in order to avoid a trivial parity effect. Otherwise, one particle survives - we would see simple diffusion of this particle on the long run (This parity effect is absent in the mean-field approximation).

Now we write down a master equation for the probability $P(\{\tau_i\})$, as done in [5]. At first, we define operators ν_i and c_i via

$$\nu_i P(\ldots, \tau_i, \ldots) \;\; = \;\; \tau_i P(\ldots, \tau_i, \ldots)$$

$$c_i P(\ldots,\tau_i,\ldots) \;=\; P(\ldots,1-\tau_i,\ldots),$$

a projection state $Q(\{\tau_i\}) \equiv 1$ and an Ising-like operator $s_i = 1-2\nu_i$ yielding -1 for an occupied site and +1 for an empty site. The master equation reads $\partial_t P = \mathcal{M} P$ with the master operator

$$\mathcal{M} = \sum_i \left(c_i c_{i+1} - 1\right)\left(\nu_i + \nu_{i+1}\right). \tag{9}$$

It describes the exchange process $01 \leftrightarrow 10$ and the annihilation process $11 \to 00$. The particular ratio between the exchange rate and the annihilation rate allows for a quadratic representation in terms of fermionic operators but does not constitute a special case since the ratio of both rates is not conserved under renormalization [4]. We introduce fermionic operators $a_i = \ldots \cdot s_{i-3}s_{i-2}s_{i-1}c_i\nu_i$ and $a_i^\dagger = \ldots \cdot s_{i-3}s_{i-2}s_{i-1}c_i(1-\nu_i)$ and find for the master operator [5]

$$\mathcal{M} = \sum_i a_{i+1}^\dagger a_i + a_i^\dagger a_{i+1} - 2a_i^\dagger a_i + 2a_{i+1}a_i. \tag{10}$$

Following [12] we are able to derive the expectation value $\langle \nu_i \nu_{i+1} \rangle$:

$$\langle \nu_i \nu_{i+1} \rangle (t) = \langle Q | \, \nu_i \nu_{i+1} \exp\left(t\mathcal{M}\right) | P_0 \rangle \,, \tag{11}$$

where P_0 is the initial state (8). We have $\langle Q | \, \mathcal{M} = 0$ and $\langle Q | \, c_i = \langle Q |$ and therefore

$$\begin{aligned}
\langle \nu_i \nu_{i+1} \rangle (t) &= \langle Q | \, a_{i+1} a_i \exp\left(t\mathcal{M}\right) | P_0 \rangle \\
&= \langle Q | \exp\left(-t\mathcal{M}\right) a_{i+1} \exp\left(t\mathcal{M}\right) \exp\left(-t\mathcal{M}\right) a_i \exp\left(t\mathcal{M}\right) | P_0 \rangle \\
&= \langle Q | \, a_{i+1}(t) a_i(t) \, | P_0 \rangle \,,
\end{aligned} \tag{12}$$

where $a_i(t) = \exp\left(-t\mathcal{M}\right) a_i \exp\left(t\mathcal{M}\right)$. By differentiating this definition with respect to t we find easily $a_i(t) = \sum_j g_{i-j}(t) a_j$, where $g_{i-j}(t) = \exp(-2t) I_{i-j}(2t)$ is the propagator of diffusion on the 1D-lattice (I_k is a modified Bessel function of order k). Using (8) and the definition of a_i we arrive at

$$\langle \nu_i \nu_{i+1} \rangle = \sum_{j,k=1}^{L} g_{i+1-j}(t) g_{i-k}(t) \, \mathrm{sign}(k-j) (-1)^{j+k}. \tag{13}$$

In order to obtain informations about the particle density we utilize the equation of motion for the moments $\langle \nu_i \rangle \equiv n_i$ [20]:

$$\partial_t n_i = \langle Q | \, \nu_i \mathcal{M} \, | P_0 \rangle = n_{i+1} + n_{i-1} - 2n_i - 2 \langle \nu_i \nu_{i+1} \rangle - 2 \langle \nu_i \nu_{i-1} \rangle \,, \tag{14}$$

where we have used $\nu_i c_i = c_i(1-\nu_i)$ and $\langle Q|\, c_i = \langle Q|$. Together with (13) we get

$$\begin{aligned}\partial_t n_i &= n_{i+1} + n_{i-1} - 2n_i - 2e^{-4t} \sum_{j,k=1}^{L} \left(I_{i+1-j}(2t) - I_{i-1-j}(2t)\right) I_{i-k}(2t) \\ &\quad \times \mathrm{sign}(k-j)(-1)^{k+j} \end{aligned} \tag{15}$$

and with the help of $I_{k-1}(2t) - I_{k+1}(2t) = (k/t)I_k(2t)$ and after (anti-) symmetrizing $j \leftrightarrow k$

$$\partial_t n_i = n_{i+1} + n_{i-1} - 2n_i + \frac{e^{-4t}}{t} \sum_{j,k=1}^{L} |k-j| I_{i-j}(2t) I_{i-k}(2t) (-1)^{j+k}. \tag{16}$$

We are now in a position to perform the continuum limit. We replace the discrete position i by a continuous variable x and the discrete Laplacian by its continuum version. Furthermore, we approximate the discrete propagator of diffusion $e^{-2t} I_{i-j}(2t) \approx (4\pi t)^{-1/2} \exp(-x^2/(4t))$, valid for $\sqrt{t} \gg L$ and $j = 1 \ldots L$. We have $\sum_{j,k=1}^{L} |k-j|(-1)^{j+k} = -L$ for L even [21] and obtain

$$\partial_t n(x,t) = \partial_x^2 n(x,t) - \frac{L}{4\pi t^2} \exp\left(-\frac{x^2}{2t}\right). \tag{17}$$

As before, we find a scale-invariant solution with the ansatz $n(x,t) = \varphi(x/\sqrt{t})/t$ ($r = x/\sqrt{t}$ is again the rescaled position):

$$\partial_r^2 \varphi + \frac{1}{2} r \partial_r \varphi + \varphi - \frac{L}{4\pi} \exp\left(-r^2/2\right) = 0, \tag{18}$$

yielding

$$\varphi(r) = \frac{L}{4\pi} \left(e^{-r^2/2} + \frac{r}{2} e^{-r^2/4} \int_0^r dy\, e^{-y^2/4} \right). \tag{19}$$

Figure (1) shows the exact profile φ for the one dimensional problem and in addition the corresponding mean-field profile, given by an appropriate numerical solution of the nonlinear differential equation $\phi'' + (r/2)\phi' + \phi - \phi^2 = 0$. We have adjusted L that both curves have the same integral. Both, the stochastic $A + A \to$ inert reaction in 1D with an initially localized configuration of particles and its mean-field approximation do in fact share the same scaling exponents. We find scale-invariant profiles $n(x,t) = \phi^*(x/\sqrt{t})/t$, and a total number of particles decaying like $N \sim t^{-1/2}$. The rescaled profiles ϕ, however, show significant differences. The exact profile has a *quartic* maximum $\phi(r) \propto 1 - r^4/24$, whereas the mean-field profile has a quadratic maximum $\phi(r) \propto 1 - 0.31 \times r^2$. Correlations between different particles, which are

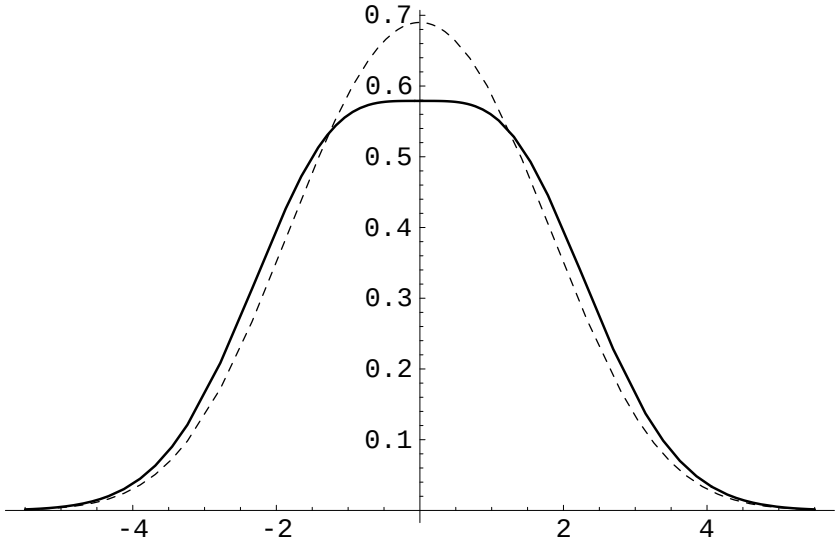

Figure 1: Exact rescaled density profile $\phi(r)$ (solid), mean-field density profile (dashed - both for one spatial dimension).

neglected in the mean-field approach, are responsible for the difference. For dimensions $d < 2$ strong anticorrelations between particle positions develop with time [22], since two adjacent particles will recombine with high probability. Therefore we have a central region with large voids and a relatively low density of particles and a number of particles, which have escaped the reaction zone.

The accuracy of the mean-field approximation generally improves with increasing spatial dimension, leading to the conjecture, that the mean-field approximation predicts the correct scaling exponents of the spreading colony also for dimensions $1 < d \leq 2$ (for dimensions $d > 2$ mean field is assumed to be correct anyway).

To conclude, we have studied the stochastic $A + A \rightarrow$ inert-reaction and have demonstrated that the mean-field approximation (2) performs well for a particular initial condition. If the particles are located initially in a small region in space from which they start to spread out, the mean-field approximation apparently predicts the correct scaling exponents of the density profile due to the fact, that the renormalization of the $A + A \rightarrow$ inert-reaction is quite primitive - only the reaction rate but not the propagator is getting renormalized [4, 17]. This should be contrasted to the homogeneous case, where mean-field (2) is wrong [23] for $d \leq 2$. Of course, in the homogeneous case, the mean-field equation does not know anything about diffusion, whereas in the spatially inhomogeneous case the diffusion term is important.

Comparing the exact density profile for $d = 1$ with its mean-field approximation, we find significant differences and show that stochastic fluctuations are still relevant. It would certainly be interesting to see wether other systems with similar RG-properties like the multi-species reaction scheme [24] display analogous features.

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